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Note

Critical points in electron – Zn atom elastic scattering

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Abstract : Partial wave method along with a complex, energy dependent, local and central optical potential is employed to get the critical points for the electron – Zn atom elastic scattering. At critical points E_c = 486.3 eV and Θ_c = 124.5°, the differential cross section attains a value of $4.488 \times 10^{-6}\ a_0^2\mathrm{Sr}^{-1}$. About 80% spin polarization of scattered electron beam is obtained at angles 124.1° and 124.8° for the critical energy E_c.

Keywords : Critical points, electron, Zn atom, differential cross section, spin polarization.

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It is now well-established that the differential cross section (DCS) for the elastic scattering of electrons by heavier atoms, when plotted as a function of scattering angles, exhibits marked structures. An interesting feature of these structures in DCS is the presence of the critical points (E_c, Θ_c) defined as a pair of the energy and the angle at which the DCS attains its smallest value with respect to incident energy and scattering angle [1]. The region, where well-defined minima in the DCS occurs, depends upon the atomic number Z and extends from a few eV upto several hundreds of eV. The interest in critical points ensues from the fact that if an unpolarized beam of electrons with incident energy E_c is scattered elastically by a heavier atom, the beam of the scattered electrons is highly spin-polarized at the scattering angles close to Θ_c. Further, knowledge of the critical points and spin polarization is essential for the complete understanding of the elastic scattering of electrons by atoms. In view of the numerous applications of polarized electrons [2,3], their study becomes exceedingly important particularly, in their scattering from heavier atoms.

In the past years, a lot of theoretical and experimental work on DCS for elastic scattering of electrons by a large number of targets have been reported. However, a limited number of investigations [2,4–12] are available on critical points and spin polarization. Recently, Sienkiewicz *et al* [13] have calculated the critical points for the elastic scattering of electrons by Zn (Z = 30) atom. They have solved relativistic Dirac-Fock equation, for a small energy range of 10 eV to 40 eV, by taking static field, exchange, polarization and spin-orbit interactions. They have neglected the absorption effects. The values of critical points obtained by them are E_c = 26.0 eV and Θ_c = 116° and the highest degree of spin polarization obtained in the vicinity of Θ_c is 15%. As a matter of fact, a highly spin-polarized beam of scattered electrons is expected at angles close to Θ_c. A low value (15%) of spin polarization obtained by Sienkiewicz *et al* [13] suggests that the reported values of critical points by them may not be the correct pair of critical points. Hence, it is worthwhile to reinvestigate the critical points for the elastic scattering of electrons by Zn atom by considering wider range of incident electron energies.

In the present investigation, we have employed the method of partial waves along with an optical potential which comprises of the direct static, dynamic polarization, local exchange, absorption and spin-orbit interaction potentials. The critical points obtained in the present

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investigation differ completely from the Sienkiewicz *et al* [13] values and show about 80% spin polarization at angles close to critical angle. Further, the order (10^{-6}) of minimum differential cross section obtained in the present investigation at Θ_c is much smaller than the order (10^{-2}) obtained by Sienkiewicz *et al* [13].

To get the critical points, we require the differential cross section (DCS)/I (E,Θ), for an unpolarized beam of electrons scattered elastically by Zn atom. In the static field-polarization-exchange-absorption and spin-orbit approximation the I (E,Θ) and the Sherman function $S(\Theta)$, that determines the degree of spin polarization of the scattered electron beam, are given by

$$I(E),\Theta) = |f(\Theta)|^2 + |g(\Theta)|^2 \tag{1}$$

and

$$S(\Theta) = \frac{f(\Theta)g^*(\Theta) - f^*(\Theta)g(\Theta)}{I(E,\Theta)} \tag{2}$$

where $f(\Theta)$ and $g(\Theta)$, respectively, are the direct and spin flip scattering amplitudes and can be obtained from the following expressions [8]

$$f(\Theta) = \frac{1}{2ik}\sum_{l=0}^{N}\Big[(l+1)\left\{\exp\left(2i\delta_l^{l+1/2}\right)-1\right\}$$

$$+l\left\{\exp\left(2i\delta_l^{l-1/2}\right)-1\right\}\Big]P_l(\cos\Theta) + f_{dp}^{B}(\Theta)$$

$$-\frac{1}{k}\sum_{l=1}^{N}(2l+1)\delta_l^S P_l(\cos\Theta) \tag{3}$$

and

$$g(\Theta) = \frac{1}{2ik}\sum_{l=1}^{N}\Big[\exp\left(2i\delta_l^{l+1/2}\right)$$

$$-\exp(2i\delta_l^{l+1/2})\Big]P_l^1(\cos\Theta), \tag{4}$$

where k is the magnitude of the momentum vector of the incident electron of energy E, $P_l(\cos(\Theta))$ and $P_l^1(\cos\Theta)$ are respectively, Legendre and associated Legendre polynomials $f_{dp}^{B}(\Theta)$ and δ_l^S are respectively, the first Born scattering amplitude and semi-classical phase shifts for the long-range polarization potential. N is an integer such that for the N-th parital wave, the exact phase shifts δ_l^j are within 2% of the δ_l^S. If this condition is not satisfied at any energy, the maximum value of N = 30 is taken. δ_l^j are the phase shifts for $j = l \pm \frac{1}{2}$ and these phase shifts were obtained by solving the following radial differential equation under appropriate boundary conditions (atomic units have been used where length is expressed in terms of a_0 and energy in Rydberg)

$$\left[\frac{d^2}{dr^2} + k^2 - V_{opt}(r) - \frac{l(l+1)}{r^2}\right]U_l(r) = 0, \tag{5}$$

where $V_{opt}(r)$ represents an optical potential, which in general is a complex, non-local, non-spherically symmetric and depends on the energy of the incident electron. However, in the present investigation, we have taken it as a complex, localized, energy and spin-dependent spherically symmetric potential given by

$$V_{opt}(r) = V_{ds}(r) + V_{dp}(r) + V_{ex}(r)$$

$$+V_{so}(r) + iV_{abs}(r) \tag{6}$$

For the direct static potential, $V_{ds}(r)$, and the electron density function $\rho(r)$, we have used the analytical expression of Salvat *et al* [14] given by

$$V_{ds}(r) = -\frac{2Z}{r}\sum A_i \exp(-\alpha_i r) \tag{7}$$

and

$$\rho(r) = \frac{2Z}{4\pi r}\sum A_i\alpha_i^2 \exp(-\alpha_i r), \tag{8}$$

where the parameters α_i and A_i are tabulated in Salvat *et al* [14]. $V_{ex}(r)$, in eq. (6), is the asymptoticallyadjusted free electron gas exchange potential of Riley and Truhlar [15] and is given by

$$V_{ex}(r) = -\frac{4}{\pi}k_F \quad \frac{1}{2} + \frac{1-\eta^2}{4\eta} + \ln\frac{1+\eta}{1-\eta} \tag{9}$$

where fermi momentum

$$k_F = \left[3\pi^2\rho(r)\right]^{1/3},$$

$$\eta = \frac{S}{k_F}$$

and

$$s^2 = k^2 + k_F^2.$$

The polarization potential is represented by the energy - dependent and spherically symmetric potential of Jhanwar and Khare [16] given by

$$V_{dp}(r) = -\frac{\alpha_d r^2}{\left(r^2+d^2\right)^3} - \frac{\alpha_q r^4}{\left(r^2+d^2\right)^5} \tag{10}$$

with

$$d = \frac{3k}{4\Delta},$$

Here α_d and α_q are, respectively, the dipole and quadrupole polarizabilites of the Zn atom. Δ represents the mean excitation energy and is given as

$$\Delta = \exp\left[L(-1)/S(-1)\right], \tag{11}$$

where $L(-1)$ and $S(-1)$ are dipole sums and require the dipole oscillator strength distribution for their determination [17]. To calculate Δ we have used $L(-1) = -1.545$ and $S(-1) = 8.362$ [18] and obtained $\Delta = 0.831$. For the spin-orbit interaction potential we have used

$$V_{so}(r) = \xi(j,l)\frac{\alpha^2}{2}\frac{d}{dr}\left[V_{ds}(r) + V_{dp}(r) + V_{ex}(r)\right]. \tag{12}$$

α is fine structure constant and

$$\xi(j,l) = \frac{l}{2} \quad \text{for} \quad j = l + \frac{1}{2},$$

$$\xi(j,l) = -\frac{l+1}{2} \quad \text{for} \quad j = l - \frac{1}{2}.$$

It may be noted that $V_{so}(r)$ aslo arises when the Dirac equation for a central field is recast as an equivalent Schrödinger equation for the large components of the relativistic wave function.

For the absorption potential $V_{abs}(r)$, we have employed absorption potential of Staszewska *et al* [19] which is given by

$$V_{abs}(r) = -\frac{8\pi\rho(r)T_{loc}^{1/2}}{5k^2}X$$

$$X = k_F^{-3}H(x)(A_1 + A_2 + A_3) \tag{13}$$

with

$$A_1 - \frac{5k_F^3}{}$$

$$A_2 = -k_F^3\left(5k^2 - 3k_F^2\right)\left(k^2 - k_F^2\right)^{-2}$$

$$A_3 = 2H(y)y^{5/2}\left(k^2 - k_F^2\right)^{-2},$$

$$x = k^2 - k_F^2 - \Delta,$$

and

$$x = 2k_F^2 + \Delta - k^2.$$

T_{loc} is the local kinetic energy of the incident electron, $H(x)$ is Heaviside unit step function.

To search the deepest minima in the DCS with respect to the incident energy and the scattering angle, we have solved the radial differential eq. (5) for a large number of energies varying from 25 eV to 650 eV and phase shifts have been obtained. These phase shifts are used to calculate and $f(\Theta)$ and $g(\Theta)$ hence differential cross section $I(E,\Theta)$ and the Sherman function $S(\Theta)$(eqs. 1 and 2). The study of calculated DCS results reveals that the deepest minima (4.488 x 10–6 $a_0^2Sr^{-1}$ in the differential cross section occurs at energy E = 486.3 eV and scattering angle Θ = 124.5° (see Table 1). The values of DCS and the $S(\Theta)$ for this energy at two different scattering angles where $S(\Theta)$ attains its maximum value (positive or negative) close to the critical angle are also given in Table 1. To see the effect of the change in incident energy on the minimum value of DCS, the results for the energies 486.1 eV, 486.2 eV, 486.4 eV and 486.5 eV are also given in Table 1.

It is evident from Table 1 that at incident energy E = 486.3 eV and angle 124.5°, the spin polarization of the scattered electron beam is only 15%. However, about 80% spin polarization of the scattered electron beam occurs at angles 124.1° and 124.8°. These angles lie on both sides of the angle 124.5°, where the DCS attains its smallest

Table 1. Values of differential cross sections, $I(E,\Theta)$, and Sherman function, $S(\Theta)$, for electron – Zn elastic scattering.

E (eV)	Θ (deg.)	DCS ($a_0^2Sr^{-1}$)*	$S(\Theta)$
	124.1	9.322(−6)	−0.7771
486.1	124.5	4.685(−6)	0.1192
	124.8	8.740(−6)	0.7790
	124.1	8.975(−6)	−0.7948
486.2	124.5	4.520(−6)	0.1435
	124.8	8.679(−6)	0.7929
	124.1	8.950(−6)	−0.7964
486.3	124.5	4.488(−6)	0.1472
	124.8	8.653(−6)	0.7973
	124.1	8.972(−6)	−0.7954
486.4	124.5	4.499(−6)	0.1440
	124.8	8.650(−6)	0.7958
	124.1	9.105(−6)	−0.7665
486.5	124.5	4.547(−6)	0.0914
	124.9	1.141(−5)	0.7601

* Number in parentheses indicate powers of 10.

value. From the table, it is also clear that the depth of the minima decreases with the change in either E = 486.3 eV or Θ = 124.5°. Therefore, the energy E = 486.3 eV and the scattering angle Θ = 124.5° represent the pair of critical points (E_c, Θ_c) for the electron – Zn elastic scattering. The above analysis confirms that if the unpolarized beam of electrons of energy E_c is scattered elastically with Zn atoms, a highly spin polarized beam of scattered electrons can be obtained at angles close to the critical angle.

Sienkiewicz *et al* [13] have solved a relativistic Dirac-Fock equation to calculate the critical points for electron – Zn elastic scattering. They have considered a small energy range *i.e.* 10 eV to 40 eV and neglected absorption effects. The values of the critical points obtained by them are E_c = 26.0 eV and Θ_c = 116° and the depth of the minima at Θ_c is 2.5×10^{-2} $a_0^2 Sr^{-1}$. The highest degree of spin polarization obtained by them in the vicinity of Θ_c is 15%. A comparison of the present results with their values shows that the present value of DCS minima (4.488×10^{-6} $a_0^2 Sr^{-1}$) at Θ_c = 124.5° and E_c = 486.3 eV is ~10 times^4 smaller than the value obtained by Sienkiewicz *et al* [13] and the highest degree of spin polarization (80%) obtained in the present investigation is about 5 times larger than their value (15%). Therefore, the values E_c = 26.0 eV and Θ_c = 116° of Sienkiewicz *et al* [13] may not represent the critical points for the elastic scattering of electrons by Zn atom. Finally, to confirm the exact location of the critical points, a complete experimental study, covering a wide energy region, is warranted for the electron – Zn atom elastic scattering.

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